Summary of
Short-Range Dispersion Modeling Workshop
Cosponsored by the California Energy Commission and the California Air Resources Board

Workshop Held on
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1. INTRODUCTION

1.1. Workshop Purpose

On January 24 and 25, 2002, the California Energy Commission and the California Air Resources Board jointly sponsored a workshop on short-range (up to 10 to 20 km) dispersion modeling. The workshop's goal was to gather information that would help focus research to better assess environmental and health impacts attributable to distributed generation units and central power plants, and issues related to environmental justice. Short-range dispersion models are used extensively in assessing of the impacts and issues just mentioned. Although these models have made valuable contributions, they still need improvements.

The workshop concentrated on four major subject areas of concern:

1. Urban environment
2. Meteorology and complex terrain
3. Stable boundary layer
4. Model evaluation and database

The workshop's specific objectives were as follows:

- Identify the state-of-the-science for short-range dispersion modeling.
- Identify the short-term (one- to three-year), mid-term (three- to ten-year), and long-term (ten- to 20-year) improvements necessary for short-range dispersion models to be able to estimate hourly and annual concentrations for inert (e.g., CO, SO_2, and PM) and reactive (e.g., NO_2) pollutants.
- Estimate the cost associated with the research to improve these models.

1.2. Workshop Format

A select group of experts in the field of short-range dispersion modeling was invited to participate in the workshop, which consisted of separate sessions for each of the four subject areas mentioned above. Dr. Steven Hanna, Mr. Joseph Scire, Dr. Akula Venkatram, and Mr. John Irwin gave the presentations for the four subject areas, respectively. Each session began with a brief (~20-minute) presentation by one of these subject matter experts, who summarized the current status of their particular subject area. Each presentation was then followed by a general discussion among all participants, who reviewed the state-of-the-science, identified shortfalls in existing methodologies, and developed a list of recommendations to remedy those shortfalls. Each presentation and discussion lasted about two-and-a-half hours.

At the end of the second day of the workshop, a draft list of recommendations was distributed to the workshop participants. The participants voted on the recommendations based on the following criteria:

- Priority (high, medium, or low)

- Timing (for the work to be conducted in one to three years, three to ten years, or ten to 20 years)
- Cost (<$250,000, $250,000–$750,000, or $750,000–$1,500,000)

Note that priority does not necessarily contradict timing. For example, it might be a high priority to conduct new field experiments, but it will take a number of years to actually plan and carry out the experiments.

The votes were tallied to determine the number of votes that each recommendation had received in each category (priority, timing, and cost). The category that received the most votes was then assigned to that recommendation. For example, if a recommendation received ten votes for high priority, two votes for medium priority, and three votes for low priority, then that recommendation was considered a high priority. When there was a tie in the voting results, the category that had a higher level of urgency or expenditure was selected. For example, if a recommendation received five votes for short-term, five votes for mid-term, and two votes for long-term, then that recommendation was classified as short-term. Participants reached a consensus in most cases, i.e., more than half of the participants voted on the same category. This was especially so for the high- and medium-priority categories.

Section 2 of this report describes the presentation, research shortfalls, and recommendations for each subject area. Section 3 provides a summary of general recommendations. Section 4 presents the conclusions. Appendix A lists the workshop participants, and Appendices B through E contain the four presentations that were given at the workshop.

2. CURRENT STATUS, RESEARCH SHORTFALLS, AND RECOMMENDATIONS FOR THE MAJOR SUBJECT AREAS

This section summarizes the current status, the shortfalls identified in the current methodologies, and the recommendations for each subject area.

2.1. Urban Environment

Most existing models treat dispersion in urban environments in a simplistic manner, because many issues involved in accurately modeling transport and diffusion in urban environments are as yet unresolved. Some researchers have suggested that measurements at the standard 10-m meteorological towers are not adequate for urban environments and suggest that additional measurements should be taken above the urban canopy. The transition between the rural and the urban boundary layers is also not very well understood, and this understanding is fundamental for the development of technically sound models.

There are essentially two approaches to modeling urban environments. The first (and simpler) approach parameterizes the urban canopy with revised similarity theories. The second approach explicitly resolves obstacles (or buildings) and typically requires computational fluid dynamics (CFD) techniques, and thus, much more computational resources. The first approach is probably more practical for typical regulatory applications, but inevitably entails gross generalizations and parameterizations. The second approach is much more specific to a particular urban setting and can provide answers at the building scale (~100 m). However, the downside of this approach is that it requires significant technical expertise and resources.

2.1.1. Urban Environment State-of-the-Science Summary

Dr. Steven Hanna of George Mason University summarized the state-of-the-science for the urban environment. His presentation (included as Appendix B and summarized below) addressed scenarios of interest, the current state-of-the-science, the shortfalls of the existing mechanisms, and a work plan for improvements.

It is important to distinguish among various spatial scales of interest when modeling the urban environment, because different scales require different modeling approaches. Some of the scales include: the building scale (~100 m), the neighborhood scale (~1 km), and the urban scale (~10 km). (Note that the research community has not yet reached a consensus regarding the definitions of these various spatial scales.) The release scenarios can be routine (e.g., pollutants from mobile and stationary sources) or accidental (e.g., industrial accidents or terrorist attacks).

The older generation of urban models primarily uses Gaussian formulation with an urban version of the dispersion coefficients. These models usually do not explicitly treat the atmospheric boundary layer as altered by the underlying urban environment.

The newer generation of urban models, on the other hand, explicitly accounts for the urban boundary layer by including parameters such as the friction velocity, Monin-Obukhov length, surface roughness, displacement length, turbulence profiles, and Lagrangian time scale profiles. Some dispersion models also account for urban roughness sublayer.

In terms of modeling approaches, the newer urban models can be classified as Gaussian plume, Gaussian puff, Lagrangian particle, Eulerian grid, and computational fluid dynamics (CFD). Some models also use morphology data to characterize buildings in urban environments. The data can be as simple as the representative building height, the standard deviation of building heights, and the ratio of the building frontal area to the lot area; or as complicated as digitized building data at 1-m spacing. It is clear that simple Gaussian models can produce only gross average predictions, whereas CFD models can produce detailed predictions—for example, at various locations surrounding a building. Therefore, it is important to first clearly define the overall modeling goal, which then determines which modeling tools are appropriate for a particular application.

Dispersion model results are highly dependent on meteorological inputs. Wind fields in an urban environment are inevitably quite complex, because of buildings or other obstacles. These wind fields can be estimated by meteorological models based on limited measurements. Meteorological or wind-field model can be diagnostic and prognostic (see Section 2.2.1 for more details). Most current urban models accept the gridded meteorological fields that are estimated by external wind-field models. CFD models, on the other hand, create their own flow fields internally. An increasingly popular approach is to link meteorological models of different scales to obtain detailed urban flow conditions. For example, a coarser-resolution model will provide the initial and boundary conditions for a finer-resolution model. This finer-resolution model will then provide the initial and boundary conditions for an even finer-resolution model.

Urban modeling is a more difficult problem than traditional dispersion modeling over flat terrain, because of the uncertainty resulting from complex flow fields. There are still a number of shortfalls in existing mechanisms for modeling urban environments. As a result, our expectations of superior urban model performance probably should be lowered. The following issues represent some problems presented by urban modeling:

- Meteorological measurements are usually available only outside an urban area, and as a result, it is not clear how to infer the structure of the urban boundary layer based on these offsite data. Even when the data are measured in an urban area, the representativeness of those data is questionable.
- Database information on urban buildings is difficult to collect, archive, and generalize.
- CFD models can provide detailed solutions around obstacles; however, they require much more human and computational resources.
- Many recent field experiments show strong vertical mixing in building wakes, a phenomenon not accounted for by most current models.
- Many urban areas are characterized by urban heat island effects, which will alter the boundary layer structure, but anthropogenic heat flux is difficult to estimate.

At the end of his presentation, Dr. Hanna recommended that the California Air Resources Board participate in the analysis of the 2000 Salt Lake City field experiment data and help plan the Oklahoma City field experiment scheduled for 2003. Dr. Hanna pointed out that regardless of which modeling approach is used, better estimates of plume transport speed profiles, turbulence profiles, and Lagrangian time scale profiles in the urban boundary layer are essential.

2.1.2. Urban Environment Shortfalls Identified

After Dr. Hanna's presentation, the workshop participants reached a consensus on the following shortfalls in the current urban environment modeling approaches.

1. Turbulence scales are different between rural and urban areas, and those for urban areas are not well known. It is unclear whether the urban turbulence scales are affected by the building scales. Furthermore, the turbulence generation mechanisms (mechanical and thermal) for urban areas are different from those of rural areas, thus requiring additional consideration.
2. Because of the lack of onsite data, it is often necessary to estimate the boundary layer structure over an urban area by using the wind and stability information from a nearby rural area. The appropriateness of this approach is in question.
3. In many cases in California, urban environments cannot be treated separately from other issues such as complex terrain. An integrated approach is often lacking.
4. The treatment of the land-sea interface in most models still needs improvements. This factor is important because the majority of the California population lives within 100 km of large water bodies.
5. Wind observations in urban environments are rarely representative. There is a need for local measurements. For example, in the Salt Lake City experiment, researchers put roughly ten wind anemometers in a street canyon to measure local meteorology with sufficient detail. It is not expensive to set up a sonic anemometer at a local site. However, in a distributed generation setting with many 1-MW units, it is still probably not practical to collect local meteorological data for each of these smaller units. A formal framework should be developed to design the optimal monitor placement.
6. The final modeling products are often population exposure estimates, where sub-grid variability is also an important issue. Robust approaches to addressing sub-grid variability are still lacking. There is a need to study whether a probabilistic approach should be adopted.
7. Models often do not make the best use of available observations.
8. There are many complexities and uncertainties involved in dispersion modeling, such as those due to the complex flow structure and unique building morphology, associated with an urban environment. Therefore, it may be necessary for

modelers and decision makers that rely on model results to relax their expectations of these models. Also, a consistent framework for assessing model uncertainty and variability does not really exist. (See Section 2.4.1 for the definitions of *uncertainty* and *variability*.)

9. It is still a challenge to characterize an urban environment through factors such as the anthropogenic heat flux, variations in building morphology, and exchange between buildings/subways and the open atmosphere. Researchers need to determine situations where detailed building morphology information is not necessary.
10. The evaluation of urban models might involve different requirements than those for rural models. A consensus on the evaluation procedures for urban models is not yet available.
11. One common characteristic of recent urban field experiments, such as the 2001 Los Angeles and 2001 San Diego (Barrio Logan) experiments, is that there is strong vertical mixing in building wakes. As a result, models tend to overpredict concentration or underpredict mixing in those areas. Furthermore, many urban models do not account for the nearly calm street-level conditions often present in deep street canyons between skyscrapers.
12. Are CFD models useful in studying urban environments? More studies are needed on the parameterization of sub-grid turbulence, the parameterization of ambient turbulence, and the specification of the boundary conditions.

2.1.3. Urban Environment Recommendations

After the above shortfalls had been identified, the workshop participants then developed a list of specific recommendations to address these shortfalls.

These recommendations are summarized below in the order of priority according to the voting results. The voting results for the timing and cost ranges are also included. See Section 1.2 for a detailed description of the definitions of priority, timing, and cost, and for how the voting results were processed. Note that the order of recommendations within each priority group does not imply the order of importance.

<u>High Priority</u>

1. *Literature Review* (Timing: short-term; Cost: low).
Perform a critical literature review of the state-of-the-science for urban dispersion modeling and determination of factors for urbanization. Rank order these factors if appropriate. The review should also summarize available datasets, mainly in the United States, Europe, and Japan. Evaluate the quality of existing datasets within the context of this workshop's purposes (e.g., siting and licensing for distributed generation, environmental justice, and risk assessment). Publish the findings in a series of papers in a peer-reviewed journal such as *Atmospheric Environment.*

2. *Evaluation of Current Models* (Timing: short-term; Cost: low).
Assess current models to see how well they address short-range, urban dispersion modeling needs. Run models with field datasets of different scales to determine which models work best for each application. Identify model deficiencies, e.g., underpredicted mixing in building wakes. Consider the feasibility of various modeling methodologies (e.g., Gaussian, Eulerian grid, CFD, and physical) for different scales of problems. Classify cities in California, and perform studies for each city class.

3. *New Field Studies* (Timing: mid-term; Cost: high).
Conduct new field studies in major cities of California with mesoscale and microscale meteorological networks. Assess impacts attributable to individual distributed generation units. Develop new model algorithms based on these new field data.

4. *Building Morphology Information* (Timing: mid-term; Cost: medium).
Develop and validate building morphology for cities. Identify the level of detail required for the morphology information at different modeling scales.

5. *Urban Wind Modeling Improvements* (Timing: mid-term; Cost: high).
Improve existing urban wind flow estimation capability. This task is crucial for researchers to be able to accurately estimate dispersion.

6. *Concentration Fluctuation PDF* (Timing: mid-term; Cost: medium).
Estimate the probability density function (PDF) for concentration fluctuations at the sub-grid level. The information can be used to support a probabilistic approach in the decision making process.

Medium Priority

1. *Chemical Reaction Products* (Timing: mid-term; Cost: low).
Consider the potential impacts of chemical reaction products (e.g., formaldehyde) from distributed generation.

2. *Mobile Source Data Assessment* (Timing: short-term; Cost: low).
Assess the usefulness of other data such as the vehicle (mobile source) data for proposed distributed generation sites.

3. *Background Concentrations* (Timing: mid-term; Cost: low).
Estimate and include the background concentrations from local sources.

4. *Emissions Variability* (Timing: mid-term; Cost: medium).
The emission data for an urban environment can be extremely complex. There is a need to assess temporal and spatial variability in these emission data.

5. *Model Evaluation Methodologies* (Timing: mid-term; Cost: low).
Develop evaluation methodologies appropriate for an urban environment, including the use of suitable evaluation metrics, and procedures for data collection and analysis.

6. *CFD Modeling Feasibility* (Timing: mid-term; Cost: medium).
Evaluate the feasibility of the CFD modeling approach to determine if it can be used to create a database of turbulence data at a sub-grid level for lower-resolution models.

7. *Simple Screening Models* (Timing: short-term; Cost: low).
Develop simple screening models. The potential usefulness of these models cannot be underestimated.

Low Priority

1. *Assessment of Future City Development* (Timing: long-term; Cost: low).
Assess the future development of cities in terms of morphology, building sizes, population density, and energy use, as these changes will affect the model results.

2. *Physical Modeling* (Timing: mid-term; Cost: medium).
Perform physical modeling (e.g., wind tunnels and hydraulic flumes) to improve the understanding of dispersion issues and to validate computer models.

2.2. Meteorology and Complex Terrain

Many major cities in California are in complex terrain. Topographically forced flows, such as the drainage flow, channeling flow, downslope flow, and upslope flow, can be quite important when the synoptic forcing is weak. Because these cities are near the coast, it is essential that models also properly account for the land-sea breeze circulation. It is quite a challenge to simulate flow conditions in complex terrain under the influence of the urban and coastal environments.

2.2.1. Meteorology and Complex Terrain State-of-the-Science Summary

Mr. Joseph Scire of Earth Tech summarized the state-of-the-science for meteorology and complex terrain. Appendix C contains a copy of his presentation. Mr. Scire started by emphasizing that meteorological models provide a key set of input data, such as the wind, temperature, and mixing height fields, to dispersion models. The important features that a mesoscale meteorological model should capture include land and sea breeze circulations, upslope and downslope flows, recirculation, terrain channeling, and nocturnal jets. Spatial variability in meteorology caused by factors such as the land and water boundary, land use, terrain, soil moisture, cloud cover, and mesoscale and microscale meteorological effects is also important.

Mr. Scire compared the two major meteorological modeling approaches: diagnostic and prognostic. *Diagnostic* models analyze observations taken at discrete space and time, and do not involve any time integration. They can parameterize terrain effects such as slope flows, terrain channeling, and land and sea breezes. Diagnostic models provide three-dimensional mass consistent wind fields. They are fundamentally limited by the representativeness of the observational data set used; however, diagnostic models require much less computational resources to run than prognostic models. Requirements on the density of data needed for diagnostic model accuracy depend upon details of the site (e.g., terrain and land use) and meteorological conditions (e.g., slope flows, urban drag, and fronts).

Prognostic, or "forecast," models numerically integrate the non-linear hydrodynamic equations of motion. Prognostic models are much more computationally intensive to run than diagnostic models. They solve the basic hydrodynamic equations of motion for atmospheric flow down to resolutions of approximately 1 km. Below this resolution, it is not clear that the parameterizations of physical processes and turbulence used are appropriate. For long-term accuracy, prognostic models need to be guided by the inclusion of observations through data assimilation techniques.

Given the pros and cons associated with both types of meteorological models, Mr. Scire suggested a balanced, hybrid approach where a coarser-scale prognostic model would provide additional "pseudo observations" to a high-resolution diagnostic model. He showed a number of examples where the hybrid approach has been applied to complex terrain areas. Detailed flow features such as slope and channeling flows were realistically reproduced. However, it is recognized that most of these applications lack adequate observational datasets for verification.

2.2.2. Meteorology and Complex Terrain Shortfalls Identified

After Mr. Scire's presentation, the workshop participants identified the following shortfalls in the area of meteorology and complex terrain.

1. Observational networks of previous field studies did not adequately account for the vertical structure. Also, the horizontal resolution of observational networks was often not consistent with the local terrain gradient. More observations in complex terrain are needed.
2. The quality of diagnostic model results depend on the representativeness of the observational data. More studies are needed to determine the quantity and density of observations required for accurate diagnostic modeling. As mentioned in the above section, data requirements depend on the complexity of the site and meteorology. High-density observation data sets and data withheld schemes can be used to determine data density requirements for different scenarios.
3. Model inputs have varying degrees of quality, some of which are highly uncertain. For example, obtaining accurate soil moisture information can be quite challenging, as indicated in a recent project where researchers had to interview

the Capitol Park gardener in Sacramento about such fine details as watering times and locations.

4. It is uncertain whether models correctly characterize channeling and skimming flows in complex terrain.
5. Data from other sources such as the National Weather Service (NWS) and the Navy have not been fully explored and utilized. Also, a mechanism is needed to better distribute observational data and other numerical weather prediction (NWP) products to researchers.
6. Surface characteristics (e.g., surface roughness, soil moisture, and vegetation index) vary spatially and temporally. Researchers need to determine the level of detail (i.e., resolution) required for these data, and whether these data are available at the desired resolution.
7. Typical grid spacing used by current models may not be sufficient to characterize complex flow fields.
8. The atmospheric boundary layer may not be in equilibrium during the transition periods of sunrise and sunset.
9. There is a need to study not only the meteorology (i.e., mean flows), but also the dispersion (i.e., turbulence fields) in complex terrain. Not all meteorological models generate turbulence fields. Even for those meteorological models that do, those turbulence fields are not fully utilized by dispersion models.
10. Model sensitivity studies are often lacking because of the large computational resources required. With increasingly faster computer hardware, researchers need to conduct more sensitivity studies or consider model ensembles for uncertainty assessment. For example, the NWS is now providing operational ensemble forecasts.
11. There is a need to study how to properly characterize meteorological inputs in a coastal, complex terrain environment. For example, most models do not use cloud-type and fog data as inputs.

2.2.3. Meteorology and Complex Terrain Recommendations

The workshop participants developed a list of recommendations to address the shortfalls in existing methodologies. These recommendations are summarized below in the order of priority according to the voting results. The voting results for the timing and cost ranges are also included. See Section 1.2 for a detailed description of the definitions of priority, timing, and cost, and for how the voting results were processed. Note that the order of recommendations within each priority group does not imply the order of importance.

<u>High Priority</u>

1. *Literature Review* (Timing: short-term; Cost: low).

Perform a critical literature review on meteorology and complex terrain, similar to that discussed for urban environments in Section 2.1.3.

2. *Review of Current Datasets* (Timing: short-term; Cost: medium).
Review existing field datasets. Establish resolution requirements for input data such as soil moisture, sea surface temperature, and vegetation index. Also categorize field studies according to the valley types to systematically study channeling and skimming flows.

3. *Data Sources for Surface Characteristics* (Timing: short-term; Cost: low).
Explore all data sources for data on such features as soil moisture, sea surface temperature, and vegetation index.

4. *New Field Studies* (Timing: mid-term; Cost: high).
Conduct new tracer and meteorology field studies. Pay special attention to the horizontal and vertical resolutions in order to correctly resolve flow conditions.

5. *Model Evaluation Methodologies* (Timing: mid-term; Cost: low).
Develop proper evaluation procedures for meteorological models.

6. *Evaluation of Existing Models* (Timing: short-term; Cost: medium)
Evaluate diagnostic and prognostic meteorological models with current datasets. Identify the best models with recent datasets (e.g., the 2000 Vertical Transport and Mixing (VTMX) study in Salt Lake City, data soon to be released). Revisit historical datasets, such as the 1990 San Joaquin Valley Air Quality Study (SJVAQS) and the 1997 Southern California Ozone Study (SCOS), with the current generation of models. Also consider data to be collected in the forthcoming summer 2002 Lake Tahoe field study.

7. *Simple Screening Models* (Timing: short-term; Cost: low).
In addition to full-scale numerical models, there is also a need for simple, empirical models for screening purposes. Model performance and model complexity do not necessarily correlate directly.

8. *Model Linkage* (Timing: mid-term; Cost: medium).
Study the linkage between complex terrain and urban models, and whether a single model can treat both phenomena.

9. *Ensemble Modeling* (Timing: short-term; Cost: medium).
Conduct ensemble modeling to estimate model uncertainty, and to provide probabilistic information.

10. *Separation of Uncertainty Components* (Timing: short-term; Cost: low).
Separate different uncertainty components (e.g., uncertainty due to model inputs versus that attributable to model physics).

Medium Priority

1. *Hybrid Modeling Feasibility* (Timing: short-term; Cost: low).
Assess the feasibility of the hybrid modeling approach, which combines diagnostic and prognostic models. Prognostic models provide the first-guess fields for diagnostic models, and the latter in turn generate high-resolution wind fields to better reflect terrain effects for dispersion calculations.

2. *Treatment of Shoreline Environment* (Timing: short-term; Cost: low).
Review models for their treatment of the shoreline environment, i.e., the land-sea interface.

3. *Theoretical Study of Boundary Layer* (Timing: mid-term; Cost: low).
In addition to reviewing existing models, researchers also need to study the basic theory or physics for the evolution (i.e., non-equilibrium) of the atmospheric boundary layer at the land-sea interface.

4. *Data Access Tools* (Timing: short-term; Cost: low).
Develop tools to allow easy distribution of special and routine observational data. There are already good examples of such data access tools as the San Francisco Bay Area Mesonet Initiative (BAMI) network; the Cooperative Mesonets in Western United States (MesoWest) network, http://www.met.utah.edu/mesowest; and the Arizona Meteorological Network (AZMET), http://ag.arizona.edu/azmet/.

Low Priority

1. *Neural Network Feasibility* (Timing: mid-term; Cost: low).
Assess the feasibility of neural network modeling techniques.

2.3. Stable Boundary Layer

Basic, theoretical understanding of dispersion under stable atmospheric conditions is incomplete. The stable boundary layer (SBL) is intermittent by nature, and thus difficult to treat. Under stable, low-wind conditions, some models do not calculate impacts if the wind velocity is below a certain threshold, and in others some assumptions are made without the benefit of actual theoretical and experimental data. Under these low-wind conditions, it may be more appropriate to use puff models, rather than plume models, to model dispersion. Overall, researchers need a better understanding of how an urban area affects the SBL.

2.3.1. Stable Boundary Layer State-of-the-Science Summary

Dr. Akula Venkatram of University of California, Riverside, gave a presentation (see Appendix D) to summarize the state-of-the-science for the SBL. The presentation included a review of the structure of the atmospheric boundary layer in general, the significance of the SBL, an overview of current models for surface and elevated releases, and suggestions for future research.

Turbulence in the atmospheric boundary layer is essentially maintained by surface heating (a thermal force) and wind shear (a mechanical force). During nighttime, radiative cooling creates a stable temperature gradient extending from the surface. This activity leads to the development of the SBL, where turbulence generated by wind shear is suppressed by the stable temperature gradient. As a result, turbulence levels are generally one order of magnitude smaller than they are during daytime, and turbulence can be quite intermittent. Turbulence levels in the SBL are not vertically uniform, and generally decrease with height. For elevated releases, because vertical plume spread is limited, maximum concentration can occur under elevated terrain, high wind shear, or coastal fumigation conditions.

Turbulence in the SBL is difficult to characterize and parameterize because of its intermittency. Methods to estimate the boundary layer height are generally less reliable than those schemes appropriate for convective conditions. Dr. Venkatram briefly reviewed dispersion models (empirical, similarity, and K-theory) for surface releases, and noted that there is considerable scatter between observations and model predictions. Many of these models are based on the Prairie Grass field data collected in 1956, which lacked adequate vertical resolution to resolve the important vertical turbulence structure.

Dr. Venkatram also reviewed some dispersion models for an elevated release. He stated that there is currently no satisfactory method to deal with dispersion through the depth of the SBL. As a result, one ad hoc approach is to simply interpolate between models for surface and elevated releases.

Dr. Venkatram also reviewed dispersion in complex terrain under stable conditions and identified some common characteristics: (1) the flow tends to be more horizontal in stable conditions, (2) streamlines and plume are depressed toward the hill surface, (3) vertical turbulence is enhanced, and (4) concentrations are increased over flat-terrain values. One common approach is to treat the observed concentration as a weighted combination of two states: one that assumes a plume traveling horizontally around the hill, and the other that assumes a plume climbing over the hill.

In conclusion, Dr. Venkatram recommended that there is a great need for more comprehensive field experiments (than, for example, the classic Prairie Grass study), which should measure information such as the vertical concentration profile. New models for dispersion through the depth of the SBL should be developed. Finally, Dr. Venkatram noted that more robust evaluation methods are necessary to distinguish between models.

2.3.2. Stable Boundary Layer Shortfalls Identified

The workshop participants identified the following shortfalls in the area of the stable boundary layer (SBL).

1. There is a dearth of information on subjects such as the vertical turbulence structure, mixing depth, horizontal mixing, temporal variation (intermittency), and nocturnal jets in the SBL.
2. A consensus is lacking on the definition of what constitutes an "urban environment" (i.e., the criteria necessary for the SBL to be considered "urbanized").
3. There is a need for high-quality flat terrain field programs to study the basic SBL structure. Because of their high quality, the Prairie Grass field data, collected in 1956 at O'Neill, Nebraska, are still being used by researchers today. However, more relevant data can be measured with state-of-the-art instrumentation. As a result, researchers would need something like the "Grandson of Prairie Grass" field trials, which will provide the impetus to study the basic SBL structure for many years to come.
4. Study of the SBL is often difficult, because the spatial variability, caused by such factors as distribution of water, irrigated crop land, and urban heat island, introduces additional uncertainty to the SBL structure.
5. Measuring turbulence aloft can be challenging. High-frequency (10 Hz) data are often required. (Tethersondes have been used in field studies in Japan and Belgium.)
6. The effects of coastal stratus, valley fog, and high cirrus on the SBL are uncertain.

2.3.3. Stable Boundary Layer Recommendations

After identifying the shortfalls, the workshop participants proceeded to develop a list of recommendations. These recommendations are grouped below according to priority, as determined by participants' voting. The voting results for the timing and cost ranges are also included. See Section 1.2 for a detailed description of the definitions of priority, timing, and cost, and for how the voting results were processed. Note that the order of recommendations within each priority group does not imply the order of importance.

<u>High Priority</u>

1. *Literature Review* (Timing: short-term; Cost: low).
Develop a survey of field studies of the SBL and urban canopy. Also review existing research on the interaction between the stable and urban boundary layers.

2. *New Field Studies* (Timing: mid-term; Cost: high).
Conduct high-quality field programs over flat terrain, using state-of-the-art equipment, to study the basic SBL structure, both horizontally and vertically.

3. *Effects of Inhomogeneity* (Timing: mid-term; Cost: medium).
Assess the effects of heterogeneous surfaces on the SBL structure.

4. *Model Parameters Selection* (Timing: mid-term; Cost: low)
Develop guidance for selecting dispersion model parameters according to the source density and turbulence complexity. Relevant model parameters include such factors as the grid size, time step, and averaging time.

5. *Review of Modeling Methodologies* (Timing: short-term; Cost: low)
Study the appropriateness of different modeling approaches, such as Lagrangian and Eulerian, for the SBL.

<u>Medium Priority</u>

1. *Theoretical Study of Development of SBL* (Timing: mid-term; Cost: low)
Develop an improved basic, theoretical understanding of the SBL.

2. *Horizontal Dispersion* (Timing: short-term; Cost: low)
Develop research on horizontal dispersion, including effects such as nocturnal jets and irrigation.

<u>Low Priority</u>

None suggested.

2.4. Model Evaluation and Database

Short-range dispersion model outputs are usually compared with field and wind tunnel data. Traditionally, data from field studies have been assumed to represent the "true" measure against which these models should be evaluated. However, this process involves problems such as the lack of enough measurements for similar meteorological situations. Similar meteorological situations can be defined as conditions with similar average winds (speed and direction) at all vertical levels, similar mixing heights, similar amount of solar radiation, similar atmospheric turbulent characteristics, and other parameters influencing the transport and dispersion of pollutants. Many data points under similar meteorological conditions are needed to estimate the statistical distribution of impacts for a given set of conditions. Because of the turbulent nature of atmospheric conditions, we cannot expect a deterministic outcome, i.e., the same concentration at a given receptor under the same meteorological and emission conditions cannot be expected. Unfortunately, field studies are extremely costly, so only a few data points can be collected under similar meteorological conditions. Therefore, it is difficult to obtain robust results by evaluating short-range dispersion models with field data. Some researchers have suggested using wind or water tunnel data instead. However, there are also questions concerning whether these laboratory data adequately replicate the true atmosphere.

2.4.1. Model Evaluation and Database State-of-the-Science Summary

Mr. John Irwin of the National Oceanic and Atmospheric Administration (NOAA), and assigned to the U.S. Environmental Protection Agency (EPA), summarized the current status for model evaluation and database (see Appendix E). He discussed the development history of air quality model evaluation methods since the 1960s. The evaluation methods evolved from simple linear regressions, to a set of common evaluation metrics, to the use of the bootstrap resampling methods to estimate the confidence limits, to a statistical procedure to estimate the robust highest concentration, to a recent standard ASTM (American Society for Testing and Materials) guide for statistical evaluation of dispersion models.

Mr. Irwin demonstrated that, if the comparison is to be paired in space, model performance is extremely sensitive to a slight shift in the predicted plume travel direction. This sensitivity suggests the uncertain nature of model evaluation and the need to separate directional errors from other types of errors.

Mr. Irwin stressed the need for an evaluation framework that tests each model's ability to perform in accordance with its designed purpose. He also noted that observations are individual realizations from an infinite ensemble; however, most dispersion models attempt to predict the average concentration for each ensemble. In terms of uncertainty and variability, the observed concentration can be envisioned as the sum of the ensemble average, instrument uncertainty, and random fluctuations; whereas the model prediction can be considered as the sum of the ensemble average, input uncertainty, and model formulation errors (e.g., due to inadequate physics).

In this context, *variability* refers to temporal and spatial differences in the value of a quantity. For example, two collocated samplers may not necessarily measure the same concentrations because of random turbulence in the atmosphere. *Uncertainty* refers to the measure of lack of complete information on a quantity. For example, model physics may be a source of uncertainty, because it is not comprehensive enough for the real atmosphere. Instrument error is another source of uncertainty. Variability is typically irreducible, whereas uncertainty is reducible. Both variability and uncertainty contribute to the disagreement between observations and model predictions. The basic philosophy for the ASTM evaluation procedure is that, due to different sources of variability and uncertainty, it is not appropriate to directly compare observations with predictions unless they are first grouped and averaged in some fashion.

In addition to the ASTM procedure, Mr. Irwin also mentioned other promising evaluation methods, such as decomposed time series and process analysis. He discussed the importance of performing scientific evaluation for models, in addition to straight statistical evaluation, because sometimes a model may give the right answer for the wrong reason, and the problem cannot be identified by a straight statistical evaluation.

2.4.2. Model Evaluation and Database Shortfalls Identified

After Mr. Irwin's presentation, the workshop participants developed and discussed the following list of shortfalls in the area of model evaluation and databases.

1. Methodologies for model performance evaluation have been relatively unsophisticated. There are no standards to gauge model performance, and evaluation procedures are often ad hoc. There is no consensus on the accepted degree of difference among models. Urban aspects of modeling, such as the plume flapping around buildings, are difficult to treat. Statisticians are rarely consulted when establishing statistical evaluation procedures. Some evaluation studies have become purely statistical exercises with no scientific insight. Researchers need to consider model evaluation in a broader context to ensure that model physics is also evaluated. A model's technical information (e.g., formulations and assumptions) is often not published on peer-reviewed literature.
2. Adequate datasets for model performance evaluation are lacking. Datasets are either of short duration with high density, or of long duration with low density, but not both. Detailed vertical profiles are almost always missing. Datasets are often not in readily accessible formats. Modelers sometimes do not carefully select databases for evaluation. In other words, the field data may not have been collected under a regime for which a model was designed.
3. A formal framework does not exist for assessing model uncertainty, and for assessing how model input errors propagate to–and manifest in–model outputs. Methodologies for detecting the relative contributions of different sources of uncertainty are also lacking. Furthermore, researchers need protocols to account for variability caused by random atmospheric turbulence. (The recently proposed ASTM procedure would be a good starting point for the development of this framework.)
4. Researchers need corresponding evaluation procedures for air quality, meteorological, and emission models. These procedures may be different.
5. Even though all models are useful in some aspects, researchers need to recognize when and why a model has limited usefulness. Researchers have primarily focused on how models succeed, but not on how they fail.
6. Adequate descriptions of a model's capabilities and limitations are not always available. That is, the "truth-in-advertising" statements for model capabilities are often missing.
7. Large-scale models are often difficult to run. As a result, sensitivity studies for these models are rarely conducted.
8. Researchers lack standard model evaluation kits similar to those distributed at the European Harmonization Workshops on atmospheric dispersion modeling (see http://www.dmu.dk/AtmosphericEnvironment/harmoni.htm).

2.4.3. Model Evaluation and Database Recommendations

As with other topics, a list of recommendations was developed by the workshop participants to address the shortfalls. These recommendations are summarized below in the order of priority, based on the voting of the workshop participants. The voting results for the timing and cost ranges are also included in parentheses. Section 1.2 provides a detailed description of the definitions of priority, timing, and cost, and for how the voting results were processed. Note that the order of recommendations within each priority group does not imply the order of importance.

<u>High Priority</u>

1. *Literature Review* (Timing: short-term; Cost: low).
Perform a critical literature review of the state-of-the-science for model evaluation, with emphasis on short-range and urban-scale modeling. This will include a critique of existing databases, modeling approaches, and model types.

2. *Specification of Evaluation Objectives* (Timing: short-term; Cost: low).
Clearly define the statistical objectives to be reached. Clearly specify the variables to consider, such as the types of outputs (e.g., arc maximum, overall maximum, cross-arc integrated, paired in space, paired in time, concentration, and dosage) and averaging time.

3. *Working Group* (Timing: short-term; Cost: low).
Establish a working group to study factors such as evaluation procedures and available datasets. EPA currently has such an internal working group. In addition to meteorologists and dispersion modelers, the working group should also include statisticians.

4. *Regular Conference Calls* (Timing: short-term; Cost: low).
Hold regular telephone conference calls among interested scientists to discuss issues regarding model uncertainty and variability.

5. *Datasets Accessibility* (Timing: mid-term; Cost: medium).
Make datasets (existing and new) easily accessible. Establish data servers (e.g., similar to dataserver.ucar.edu) to facilitate information exchange.

6. *Terminology Standardization* (Timing: short-term; Cost: low).
Develop standard terminology through, for example, the ASTM forum. There is often confusion among various disciplines regarding the definitions of terms such as *uncertainty, variability, stochastic, evaluation,* and *validation.*

7. *Model Runoff* (Timing: short-term; Cost: medium).
Hold a model runoff where a number of models are applied to the same field datasets. The runoff could also be "blind" for new datasets, where the observed concentration data are not made available to modelers at the same time as the source and meteorological data.

8. *Workshop on Model Failures* (Timing: short-term; Cost: low).
Hold a workshop on applications where certain models perform badly, e.g., poor performance for photochemical models during nighttime. It is often equally, if

not more, valuable to learn how models fail for certain scenarios as it is to learn how they succeed.

Medium Priority

1. *Stochastic Variability* (Timing: mid-term; Cost: medium).
The atmosphere is characterized by random turbulence. As a result, all measurements carry inherent variability. Researchers should develop techniques to model this stochastic variability.

Low Priority

None suggested.

3. SUMMARY OF GENERAL RECOMMENDATIONS

The preceding section describes in detail the recommendations to improve the current short-range dispersion modeling capabilities for each of the four subject areas. It is evident that there are a number of overarching issues that are common to all subject areas. These general issues are further summarized below, in order to provide clearer guidelines for improving short-range dispersion modeling capabilities.

3.1. Critical Literature Review

A common starting point for all recommendations is a comprehensive, critical literature review in order to understand the current status of all subject areas. This activity includes the review of current theories, modeling methodologies, and available datasets for model development and evaluation. This task is especially important as other research communities, such as those in Europe and at the departments of Defense and Energy, are also faced with similar challenges in short-range dispersion modeling. Moreover, the review would also help identify problems with existing models, and gaps and shortcomings in available datasets.

The literature review should also include surveys of various terrain, land use, soil moisture, surface characteristics, and building morphology databases. New, potentially valuable databases are frequently made available on the Internet; therefore, this review could capture this type of information much more easily and comprehensively than in the past.

3.2. New Field Studies

Field data are instrumental in developing and evaluating new theories and models. Well-designed field programs often lead to significant scientific progress. For example, the classic Prairie Grass experiments, conducted nearly 50 years ago, are still being used by scientists to develop or evaluate new theories. However, it is also recognized that as the instrumentation technology advances, many goals that were previously not practical to achieve are now possible. Many historical field experiments, although of high quality, were not designed specifically for the subject areas of this workshop. Moreover, most field studies were conducted over relatively horizontally homogeneous areas. This is a problem for modeling areas in California, where factors such as irrigation clearly play a role in introducing spatial inhomogeneity.

Mr. Scire presented at the workshop examples of a hybrid modeling approach, where a prognostic meteorological model is run in conjunction with a diagnostic model, for complex terrain with sparse observational data. Even though the results look realistic, adequate complex-terrain datasets are still lacking for a true evaluation of this approach.

The recent field monitoring at the Barrio Logan area in San Diego shows that high-quality data with sufficient resolution can be gathered cost-effectively.

Based on past experience, it has become clear that it is imperative for the scientists who will be using the field data to be involved in every phase of a field program. An unfortunate outcome for many historical field programs has been that the value of the data is greatly reduced due to a lack of communication between the data collectors and users. Finally, any new field experiment must have clearly defined scientific objectives and sufficient funding to allow for data analysis.

3.3. Model Evaluation

Models should be run using existing and new datasets to identify the best performing models for each application scenario. It is important to understand the basic assumptions and the range of applicability of each model, in order to avoid misapplication.

There are at least two types of model evaluation: scientific and statistical. *Scientific* evaluation involves the study of the adequacy of various physical algorithms and assumptions in the model, to find out whether they are consistent with the state-of-the-science. Scientific evaluation also ensures that the model will give the right answer for the right reason. There are, however, factors that often make scientific evaluation a challenging task. For example, many models lack peer-reviewed publications and comprehensive technical documents that describe the physics and theories implemented in the models. "Truth-in-advertising" statements for models' capabilities are also frequently missing.

Statistical evaluation involves the comparison of model predictions with observations obtained from field or laboratory experiments. Workshop participants mentioned the need to identify a common set of performance evaluation metrics, whose confidence limits can then be estimated through techniques such as bootstrap resampling. It is also recognized that the evaluation strategies and objectives might vary with scenarios. For example, because of different atmospheric dispersion characteristics, a flat-terrain field experiment and an urban field experiment will involve different evaluation procedures.

Mr. Irwin's presentation suggested a fundamental paradigm shift in statistical model evaluation. His rationale is that observations represent snapshots of ensembles, whereas most models are designed to predict ensemble averages. Therefore, observations and model predictions should not be directly compared unless some sort of grouping averaging are performed.

3.4. Improving Existing Models

After the above recommendations on literature review, new field studies, and model evaluation, the logical next step would be to use the knowledge thus gathered to improve existing models. Different scenarios and objectives would require different modeling methodologies. For example, simple, empirical screening models might be practical, powerful tools to understand the gross behavior of dispersion in urban areas. However, probably only the CFD modeling technique can predict detailed concentration fields at the street level or at various locations surrounding a building.

3.5. Uncertainty and Variability Analysis

Most dispersion models generate deterministic results. In other words, with the same source and meteorological data, a model always produces the same answer. Many workshop participants strongly suggested the need to study model uncertainty and variability. In other words, a probabilistic approach is preferred over a deterministic approach.

The difference between variability and uncertainty is further illustrated here. The wind speed measured at a location will be different from that measured at a nearby location, because of random turbulence in the atmosphere. There are also similar fluctuations temporally. As a result, there is *variability* in all wind measurements due to turbulence. However, the wind speed measured at a location is also *uncertain* because of instrument errors. There is also *uncertainty* in all physical parameterizations in the models. For example, many dispersion models account for the atmospheric dispersal of pollutants with Gaussian formulations, which obviously do not faithfully represent the actual atmosphere. Variability is usually inherent in the system and thus not reducible, whereas uncertainty can usually be reduced by better instrumentation and better physics.

It is important to establish a formal framework to assess model variability and uncertainty, and to use the information thus obtained in the decision making process. One common method to account for model uncertainty is Monte Carlo analysis, which involves the identification of the input parameters to be perturbed and their associated probability density functions. This information can usually be obtained through expert elicitation, where subject matter experts are asked their opinions on the typical uncertainty associated with various model input parameters. Ensemble modeling, a popular approach in the meteorological forecast model community to study model uncertainty, includes the use of different initial boundary conditions, boundary conditions, and physical parameterizations. Methodologies that are useful to assess variability include Lagrangian particle modeling, large eddy simulation, turbulence closure modeling, and physical (fluid) modeling.

3.6. Working Groups

All of the subject areas of the workshop require careful consideration and planning in order to make progress. It is not likely that a single government agency or research group alone will have the diverse and sufficient technical expertise required to address these issues sufficiently. Formation of working groups, consisting of subject matter experts from different affiliations, is a good way to foster information exchange and development. In addition to atmospheric scientists and dispersion modelers, it is also necessary to include experts from other fields (such as statisticians) in these working groups.

4. CONCLUSIONS

It is clear that although the workshop examined four subject areas, each of these areas are often interrelated to others. For example, an urban area might be located along the coast with deep valleys inland. Hence, the local meteorology is under the influence of many processes, including the urban environment, complex terrain, and land-sea breezes. As another example, the night-time stable boundary layer will be modified by the underlying urban heat island effects. Therefore, it is important to adopt an integrated approach that includes the interaction of various relevant processes.

Several overarching recommendations have been identified as high priority for all subject areas. These recommendations include:

1. Conduct a critical literature review of the state-of-the-science and existing datasets.
2. Conduct new, high-quality field studies to meet the current needs.
3. Evaluate existing dispersion models with existing and new datasets, and develop better model evaluation procedures.
4. Improve existing models.
5. Develop a formal framework to study model uncertainty and variability, in order to better understand the model behavior and to adopt a probabilistic approach in the decision making process.
6. Form working groups to facilitate exchange of ideas and to encourage development.

In addition to these general recommendations, there are also other, more specific recommendations, such as:

1. For the urban environment, determine the importance of building morphology and the appropriate resolution necessary to address each desired application.
2. Determine the role of the CFD models.
3. Do not underestimate the value of simple screening models.
4. Improve the current soil moisture database. For meteorological modeling, soil moisture has been identified as one of the most important parameters affecting the planetary boundary layer. However, its current database is still far from being satisfactory.
5. Conduct more theoretical studies to understand the basic structure of the stable boundary layer and the non-equilibrium nature of the atmospheric boundary layer at the land-sea interface.
6. Develop a standard terminology for model evaluation and uncertainty and variability analysis.
7. Interact with other research communities, such as the Department of Energy, the Department of Defense, the Environmental Protection Agency, and the European investigators as they are also confronted with similar challenges in short-range dispersion modeling.

APPENDIX A. Workshop Participants

More than thirty people participated in the two-day workshop, representing a wide spectrum covering federal and state agencies, industrial groups, universities, national laboratories, and commercial companies. Many of the participants are world-renowned scientists in short-range dispersion modeling. The table below lists all of the workshop participants.

Table A-1. List of Workshop Participants

Last Name	First Name	Organization
Birkinshaw	Kelly	California Energy Commission
Bohnenkamp	Carol	U.S. EPA
Bohning	Scott	U.S. EPA, Region 9, AIR-7
Bornstein	Bob	San Jose State University
Chang	Joe	TRW Systems
Ching	Jason	U.S. EPA, NERL
Du	Shuming	California Air Resources Board, PTSD
Hakkarinen	Chuck	EPRI
Hanna	Steven	George Mason University
Harris	Greg	California Air Resources Board, SSD
Hernandez	Janel	California Air Resources Board, ASD
Houghton	Michele	California Air Resources Board, SSD
Hui	Steve	California Air Resources Board
Irwin	John	Environmental Protection Agency
Isakov	Vlad	California Air Resources Board, PTSD
Koracin	Darko	Desert Research Institute
Lents	Jim	University of California, Riverside
Linden	Paul	University of California, San Diego
Long	Glen	Bay Area AQMD
Mueller	Marla	California Energy Commission
Pederson	Jim	California Air Resources Board, RD
Ranzieri	Andrew	California Air Resources Board, PTSD
Sax	Todd	California Air Resources Board, PTSD
Scire	Joe	Earth Tech, Inc.
Servin	Tony	California Air Resources Board, PTSD
Sugiyama	Gayle	Lawrence Livermore National Lab
Sykes	Ian	Titan Corporation
Takemoto	Brent	California Air Resources Board
Venkatram	Akula	University of California, Riverside
Vine	Ed	University of California, Office of President
Wang	Zion	University of California, Riverside
Wilson	Mark	Consultant to CIEE

APPENDIX B. Dr. Steven Hanna's Presentation on Urban Environment

State of the Science of Short Range Dispersion Modeling in Urban Environments

Steven R. Hanna

George Mason University
Fairfax, VA
shanna@gmu.edu

Presented at CEC/CARB Short Range Dispersion Modeling Workshop

January 24 and 25, 2002
Sacramento, CA

Modeling Scenarios of Interest

Current State-of-the-Science

Short-Falls of Existing Mechanisms

Work Plan for Improvements

Modeling Scenarios of Interest

Space scales: building, block, neighborhood, urban

Routine releases: NOx, VOC, SO_2, PM, toxics from mobile sources, industry, commercial, power plants

Accidental or terrorist: subway, in building, street canyon, elevated line source, transportation.

Current State-of-the-Science

Old models:

ISC-urban
Many Gaussian Plume Models with Briggs' Urban Sigma Curves
ATDL simple urban model
UAM
Various street canyon and line source models

Newer models:

HPAC-UDM
MIDAS-AT
AERMOD
HPDM-urban
Rotach Lagrangian particle model
Various CFD models and simplifications
NARAC
Eulerian grid models (e.g., CMAQ, CAMx, UAM-V, CALGRID, MAQSIP, …)

Urban Boundary Layer

Fluxes for inputs to mesoscale urban models

Specify u^*, L, z_o, d for estimation of profiles of winds, temps, turbulence

Above and below avg. building elevation H_r

Urban roughness sublayer
Near-constant characteristic speed u_c

HPDM urban BL model has been improved upon by Grimmond and Oke LUMPS model

Many new data bases of urban BL

Data bases of urban morphology – dimensions and locations, find that $\sigma_{Hr}/H_r \approx 0.5$ to 1.0.

Dispersion Models

Now based on new urban boundary layer models

H_r, λ_f, z_o, d, u^*, L, σ_w, σ_v, σ_u, Lagrangian time scales T_L

UDM – Allows for enhanced lateral spread by buildings, detrainment from building wakes.

Street canyon models allow for vortex, traffic-induced turbulence

Move from local street canyon scale through neighborhood scale to full urban scale

Many new laboratory and field data

Are CFD models useful? Problems with turbulence

Shortfalls of Existing Mechanisms

Given wind speed and stability outside urban area, what is BL inside?

Urban area is by definition complex; therefore no wind speed observation is representative. What is best to do?

Should building structure details be worried about?

Given all the uncertainties, should we relax expectations of models?

How can anthropogenic heat flux be determined and accounted for?

How do we account for variations in buildings?

What are mechanisms for exchanges between buildings or subways and open atmosphere?

Are CFD models useful? How can subgrid turbulence be parameterized and boundary conditions?

What about near-street level conditions in deep street canyon/skyscraper situations? Nearly-calm?

It looks like there is strong vertical mixing in building wakes.

What if rural area is very stable at night? What happens in the urban area?

Work Plan

Resolve short-fall areas from previous pages

Participate in SLC data analysis and model eval.

Help planning for OK City 2003 field study

Improvements needed in BL parameterizations at $z < H_r$

In light of uncertainties, how much detail is needed?

Do we really need multiscale linked models from building to urban scale?

Add chemistry, aerosols, Deposition.

Eulerian models with Plume-in-Grid or Lagrangian particle models?

No matter what, we need estimate of plume transport speed profiles, turbulence profiles, and Lagrangian time scale profiles

APPENDIX C. Mr. Joseph Scire's Presentation on Meteorology and Complex Terrain

Short-Range Dispersion Workshop

Sacramento, California
January 24-25, 2002

Meteorology and Complex Terrain

Presented by:

Joseph Scire
Earth Tech, Inc.
196 Baker Avenue
Concord, Massachusetts 01742

METEOROLOGICAL MODELING

- **Meteorological models provide a key set of inputs into dispersion models**
  - Wind fields
  - Temperature fields
  - Other meteorological variables
    - Mixing heights
    - Heat and momentum fluxes
    - Stability parameters
  - Spatial resolution
    - Single point values
    - Vertical profiles
    - Three-dimensional winds and temperatures, 2-D other meteorological fields

EXAMPLES OF IMPORTANT FEATURES OF FLOW FIELDS

- **Land/sea breeze circulations**
- **Upslope/downslope flows**
- **Recirculation**
- **Large eddies (Fresno, Sacramento eddies)**
- **Terrain channeling**
- **Noctural jets**

OTHER IMPORTANT METEOROLOGICAL FACTORS

- **Horizontal and vertical temperature structure (3-D field)**
- **Spatial (2-D) variability in mixing heights**
- **Spatial (3-D) changes in turbulence fields**
- **Factors leading to spatial variability**
  - Surface characteristics (land/water boundary, land use changes such as urban/rural, agricultural/forest, etc.)
  - Soil moisture variability
  - Cloud coverage
  - Terrain effects
  - Mesoscale/synoptic systems
  - Microscale effects (e.g., buildings, other structures)

PROGNOSTIC METEOROLOGICAL MODELS

- **Common features of mesoscale prognostic models include:**
  - Non-hydrostatic dynamics
  - Variety of options for boundary layer parameterizations, cloud microphysics, cumulus parameterizations, land-surface parameterizations
  - Multiple nesting options (2-way and 1-way nesting)
  - Option for four-dimensional data assimilation
- **Examples of mesoscale models**
  - MM5
  - RAMS
- **Examples of operational large-scale models**
  - ETA
  - AVN
  - MRF
  - RUC2
  - NOGAPS
  - ECMWF

DIAGNOSTIC METEOROLOGICAL MODELS

- **Observational data used to drive the model solutions**
  - Surface, upper air, precipitation stations
  - Overwater (buoy) observations
  - Geophysical data (terrain and land use)
- **Parameterized treatments of terrain effects**
  - Slope flows (upslope/downslope)
  - Terrain channeling effects
  - Kinematic terrain effects
  - Sea breeze parameterization
- **Three-dimensional mass consistency**
- **Boundary layer modules**
  - Overland boundary layer
  - Overwater boundary layer
- **CALMET is an example of regulatory diagnostic model**

PROGNOSTIC VS. DIAGNOSTIC MODELS

- **Advantages of prognostic models –**
  - Sophisticated treatment of physical processes
  - Dynamically self-consistent fields even without observations
  - Data assimilation allows some degree of consistency with observations
- **Disadvantages of prognostic models**
  - Currently cost prohibitive to run on small scales (3-5 km grid is a practical limit)
    - Example: 3 nests (60 km, 20 km, 5 km), MM5, annual simulation: 60 days CPU on workstation
  - Higher level of difficulty to run model
  - Inadequate data or data gaps may lead disagreement with observations
  - Results at finest grid scale are mixed, model refinements may be needed

PROGNOSTIC VS. DIAGNOSTIC MODELS

- **Advantages of diagnostic models –**
  - Results faithfully reflect observational data, which may include prognostic output as pseudo-observations
  - Simple parameterizations are often quite robust
  - Relatively simple to operate and run
  - Computationally efficient even for fine scale grids (grid size ~ few hundred meters)
    - Example: Annual simulation ~ 0.5 days on workstation
- **Disadvantages of diagnostic models**
  - Simple parameterizations are limited in their ability to predict complex flow features not contain in the input data
  - Depends on good quality observational data

DATA LIMITATIONS ON MODEL PERFORMANCE

- **Need balanced approach**
  - New generation dispersion models using turbulence-based dispersion coefficients require more data than previous models
    - Soil moisture
    - Land use data and terrain resolution
    - Cloud data
    - Snow cover
    - LAI
    - Sea surface temperature data
    - Time and space variability of these parameters
  - Proper grid resolution is essential, often more important than model choice
- **Model performance may often be controlled by data limitations rather than model parameterizations**
    - Effort needed improve quality of datasets

COMPUTER REQUIREMENTS

- **Model requirements include hourly and annual concentration predictions, therefore computer requirements based on annual simulations**
  - CPU requirements
    - Prognostic: ~2 months CPU time for 5 km resolution
    - Diagnostic: $\leq$ 1 day CPU time for fine resolution
  - RAM requirements
    - Prognostic: 1-4 GB
    - Diagnostic: < 1 GB
  - Disk requirements
    - 10-40 GB disk requirements

SUMMARY

- **Meteorological modeling is a critical component of the dispersion modeling process**
- **Complex wind flow features are common in modeling applications**
- **Spatial variability in meteorological fields other than winds (e.g., mixing heights, turbulence) are often significant**
- **Diagnostic and prognostic models each have strengths and limitations**
  - Transition occurring from single point met. models to diagnostic models for routine applications for scales beyond few km
  - Prognostic models will become more practical and common as computer simulation speed and model parameterizations improve
- **Hybrid (fine-scale diagnostic modeling combined with coarse scale prognostic modeling) offers practical benefits in near and intermediate terms**
- **Data limitations may restrict new-generation dispersion model performance. Efforts to improve quality of datasets should be a priority.**

APPENDIX D. Dr. Akula Venkatram's Presentation on Stable Boundary Layer

Dispersion in the Stable Boundary Layer

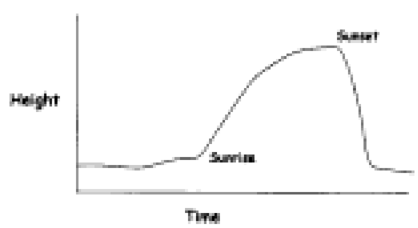
by
Akula Venkatram
University of California, Riverside

- Structure of the ABL
- Significance of the SBL
- Surface releases
- Elevated releases
- Future research

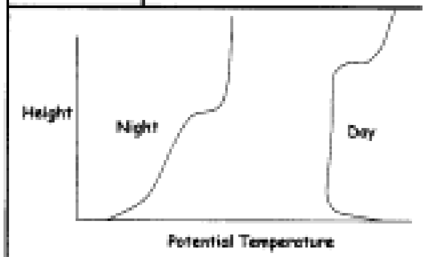
The Atmospheric Boundary Layer

- The layer next to the ground that is turbulent
- Turbulence maintained by surface heating and wind shear
- Boundary layer height varies from ~100m at night to about ~1000m during the day

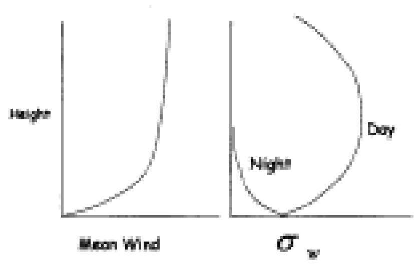
ABL Evolution



Temperature Profiles



Velocity and Turbulence Profiles



Features of SBL

- Surface radiative cooling at night creates stable temperature gradient extending from the surface
- Turbulence generated by wind shear is suppressed by stable temperature gradient
  - Turbulence levels are small~1/10 of daytime levels
  - Velocity gradients are large
- Turbulence levels generally decrease with height
- Boundary layer height determined by shear generated turbulence
  - height is typically tens of meters

Significance of SBL

- Because vertical plume spread is inhibited, concentrations can be high for
  - Surface releases
  - Elevated releases
    - elevated terrain
    - high wind shear conditions
    - Coastal fumigation
- Understanding is critical to estimating dispersion in a vertically non-uniform boundary layer

Modeling the Stable Boundary Layer

- Research conducted by Nieuwstadt, Mahrt, Wyngaard, Derbyshire
- Turbulence is intermittent and difficult to characterize
- Difficult to parameterize the structure
- Methods to estimate boundary layer height are unreliable

Surface Friction Velocity

$$u_* = \sqrt{\frac{\tau_o}{\rho_a}}$$

$$\sigma_w = 1.3u_*$$

Monin-Obukhov Length

Height at which shear production is equal to buoyant destruction

$$L = -\frac{T_o}{g}\frac{u_*^3}{kQ_o}$$

Models for the SBL

$\theta_* \sim$ constant

$L \sim u_*^2$ (Venkatram, 1980)

$z_i = Au_*^{3/2}$

$$\sigma_w = 1.3u_*\left(1 - \frac{z}{z_i}\right)^{3/4}$$

$$l = \frac{\sigma_w}{N} \quad \text{where} \quad N = \left(\frac{g}{T_o}\frac{d\theta}{dz}\right)^{1/2}$$

$$\varepsilon = \frac{\sigma_w^2}{N}$$

Surface Releases

- Parameterization of Observations- Briggs, Venkatram
- Lagrangian Similarity Theory-Horst, Meroney
- K-Theory- Van Ulden, Gryning
- Lagrangian Stochastic Modeling-Wilson, Thomson, Sawford
- Parameterization of results from LSM- Du and Venkatram

Surface Releases-Prairie Grass Data

- Project Prairie Grass was a short range dispersion experiment conducted in 1956 at O'Neill, Nebraska.
- Ground-level concentrations measured on 5 arcs ranging from 50 to 800 m.
- Vertical profiles measured only at 100 m

Semi-Empirical Models

$$u\frac{dh^2}{dx} \sim u_* L$$

$$\frac{u_* h}{L}\frac{dh^2}{dx} \sim u_* L$$

In the limit of large stability

$$h \sim x^{\frac{1}{3}} L^{\frac{2}{3}}$$

$$\boxed{\bar{C}^y \sim \frac{Q}{u_* x^{\frac{2}{3}} L^{\frac{1}{3}}}}$$

Description of Prairie Grass

$$\begin{aligned} \bar{C} &= \bar{x}^{-1} \text{ ; for } \bar{x} \le 1.4 \\ &= 0.9\bar{x}^{-4/3} \text{ ; for } \bar{x} > 1.4 \text{ for stable conditions} \\ &= \frac{1}{\bar{x}(1 + 0.006\bar{x}^2)^{1/2}} \text{ ; for } \bar{x} > 1.0 \text{ for unstable conditions} \end{aligned}$$

where

$$\bar{C} = \frac{\bar{C}^y u_* |L|}{Q} \qquad \bar{x} = \frac{x}{|L|}$$

Models- Similarity, K-Theory

$$\boxed{\bar{C}^y(z) = \bar{C}^y(0)\exp\left[-b\left(\frac{z}{\bar{z}}\right)^s\right]}$$

$$\bar{C}^y(0) = \frac{AQ}{U(x)\bar{z}}$$

Horst gives analytical expression s for s, A, b, $\bar{z}$, and U(x)

Horizontal Distribution

Distribution is taken to be Gaussian

$$\sigma_y = \sigma_v t / (1 + t / 2T_{Lv})^{1/2}$$

$$T_{Lv} = \frac{l}{\sigma_v}$$

What is l ?

The Gaps

- Vertical concentration profiles cannot be evaluated with observations
- There is considerable scatter between model results for surface concentrations and corresponding observations
- Horizontal spread shows little systematic behavior

Elevated Releases

$$\sigma_z = \sigma_w t / (1 + t / 2T_L)^{1/2}$$

Venkatram and Strimaitis (1988)

$$T_L = l / \sigma_w$$

$$\frac{1}{l} = \frac{1}{l_s} + \frac{1}{l_n}$$

$$l_s = \gamma \sigma_w / N; \quad l_n = k z_r$$

The Gaps

No satisfactory method to deal with dispersion through the depth of the boundary layer

- K-theory- *cannot be justified near the source*
- Split sigma method (Venkatram and Paine, 1984)- *semi-empirical with limited testing*
- Interpolation between surface and elevated releases (AERMOD)

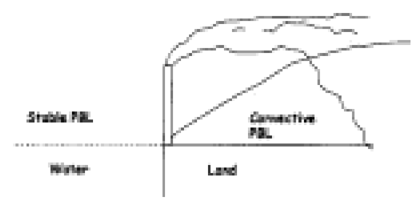
Combining Elevated and Surface Dispersion

Interpolate between surface and elevated plume spreads

$$\sigma_z^{Effective} = \sigma_z^{Elevated} .(1 - f) + \sigma_z^{Surface} .f$$

$$f = \left(1 - \frac{h_{sz}}{z_i}\right)$$

Coastal TIBL



Dispersion In Complex Terrain

- Flow tends to be horizontal in stable conditions
- Streamlines and plume are depressed towards hill surface
- Vertical turbulence is enhanced
- Concentrations are increased over flat terrain values

Approach

- Observed state is a weighted combination of two states
  - State 1 assumes that plume is horizontal
  - State 2 assumes that plume climbs over the hill

$$C(x, y, z) = fC_f(x, y, z) + (1 - f)C_f(x, y, z_e)$$

Aerosols

- Particles suspended in the air
- Vary in size from 10^-A to 100 um
- Largest settling velocities are ~ 1 m/s
  - Inertia effects: Response to velocity fluctuations
  - Trajectory crossing: Particles falling out of eddies

Inertia Effect

How well does the aerosol follow fluid motion?

$$\frac{(u_p - u_f)}{u_f} = \frac{T_{particle}}{T_{turbulence}}$$

$$T_f = \frac{l}{\sigma_w} \qquad T_p = \frac{v_s}{g}$$

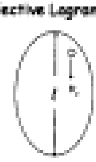
$$\frac{T_p}{T_f} = \frac{v_s \sigma_w}{g l} = 0.1$$

$$\boxed{l < 1\,m}$$

Trajectory Crossing

Particles settle out of an eddy.
For a heavy particle, the effective Lagrangian time scale is

$$T_{Leff} = \frac{l}{V_s}$$



Lagrangian Stochastic Simulation

- Simulates trajectories of particles released in a turbulent fluid
- Avoids assumptions, such as flux-gradient closure, used in earlier models
- Thomson (1987) developed method to constrain form of governing stochastic equation

Technical Approach

- Conduct simulations with Lagrangian Stochastic model for a variety of stabilities
- Evaluate model results with available observations
- Parameterize results from simulations

The Stochastic Model

$$dw = -\frac{C_0 \varepsilon}{2\sigma_w^2} w\,dt + \frac{1}{2}\left(1 + \frac{w^2}{\sigma_w^2}\right)\frac{\partial \sigma_w^2}{\partial z} dt + \sqrt{C_0 \varepsilon}\, d\xi_t$$

$$dz = w\,dt$$

$$dx = U\,dt$$

Computing Concentrations

$$\boxed{\overline{C}^y \cdot U(z) \cdot \Delta z = n/N}$$

n = Particles passing through Δz

N = Total particles released

The Parameterization

$$\boxed{\overline{C}^y(z) = \overline{C}^y(0)\exp\left[-b\left(\frac{z}{\overline{z}}\right)^s\right]}$$

$$\overline{C}^y(0) = \frac{Q}{u_e \overline{z}}$$

$$\overline{z} = 0.04x(1 + 0.24x/L)^{-1/2}$$

$$u_e = \frac{(1 + 0.26x/L)^{-1/3} u_* x}{\overline{z}}$$

Recommendations

- Need a new field study that is more comprehensive than Prairie Grass
  - Vertical concentration profile information
  - Horizontal spread
  - Vertical spread of elevated releases
- Need model for dispersion through the depth of the stable boundary layer
- Need methods to distinguish between models

APPENDIX E. Mr. John Irwin's Presentation on Model Evaluation and Database

Evaluate Earth Science Models for What They are - Cartoons of Reality

John S. Irwin, NOAA Meteorologist
EPA OAQPS
Air Quality Modeling Group
RTP, NC 27711

Model Evaluation Background

- Linear regressions (Clarke, 1964), Martin (1971).
- EPA Guideline on Air Quality Models, EPA-450/2-78-027, (OAQPS, 1978), Revised (1980, 1994, proposed 2001).
- National Commission on Air Quality Panel examines uses and limitations of air quality models, (Fox and Fairobent, 1981) BAMS(62):218-221.
- September, 1980: Woods Hole Workshop. Judging air quality model performance, (Fox, 1981) BAMS (62):499-609.
- Framework for evaluating air quality models, (Venkatram, 1982) BLM (24):371-385.

Model Evaluation Background(cont.)

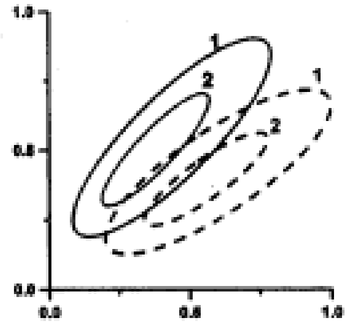
- 1984
  - Uncertainty in air quality modeling, (Fox, 1984) BAMS (65):27-36.
  - Review of the attributes and performance of 10 rural diffusion models, (Smith, 1984) BAMS (65):554-558.
  - Potentially useful additions to the rural model performance evaluation, (Irwin and Smith) BAMS (65):599-568.
- 1988: Air quality model evaluation and uncertainty (Hanna, 1988) JAPCA (38):406-412.
- 1989: Confidence limits for air quality model evaluations as estimated by bootstrap and Jackknife resampling methods. (Hanna, 1989) AE(23):1385-1398.

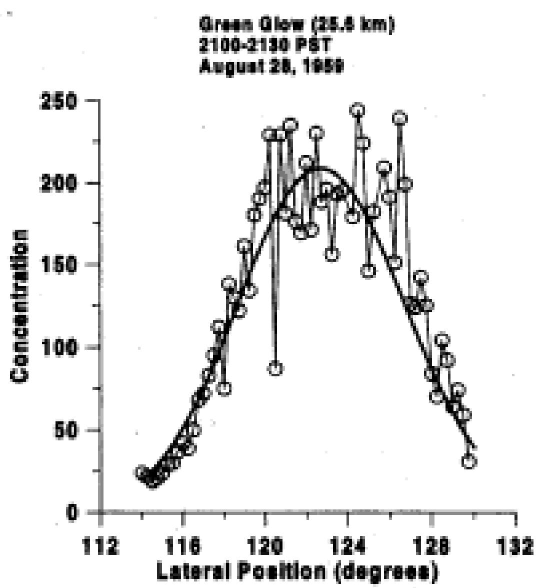
Model Evaluation Background(cont.)

- 1990: A statistical procedure for determination of the best performing air quality simulation model, (Cox and Tikvart) AE(24A):2387-2395.
- 1994: Verification, validation, and confirmation of numerical models in the earth sciences. (Oreskes et. al., 1994): Science (263):641-646.
- 2000: Standard Guide for statistical evaluation of atmospheric dispersion model performance, ASTM, D 6589-00, 16 pages.

Examples

- Examples:
  - Gaussian Plume (Irwin et al., 1987)
  - Grid Model (Hanna et al., 1998, 2001)
  - Transport Direction (Weil et al., 1992)





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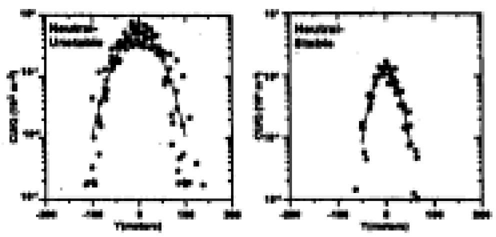
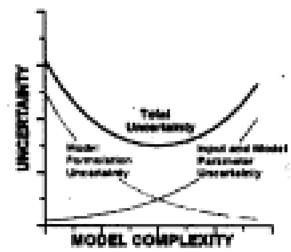
Computed correlation coefficints (r) for Run 26 Green Glow, 2100-2130 PST, August 28, 1959.

Distance downwind (m)	Displacement of peak from observed position along arc (degrees).				
	-4°	-2°	0°	+2°	+4°
800	+0.37	+0.81	+0.99	+0.83	+0.40
1,600	-0.06	+0.60	+0.94	+0.55	+0.12
3,200	-0.19	+0.56	+0.99	+0.54	+0.20
12,800		+0.06	+0.73	+0.38	
25,600		+0.39	+0.80	+0.37	

Unexplained Variability & Simple versus Complex Modeling





Evaluation

Models are "cartoons" of reality:

$$C_o(\alpha) = \overline{C_o(\alpha)} + \Delta C_o'(\alpha) + C_o'(\alpha)$$

$$C_p(\alpha) = \overline{C_p(\alpha)} + \Delta C_p'(\alpha) + C_p'(\alpha)$$

where α indicates the ensemble, $\overline{C}$ is an ensemble average, $\Delta C'$ represents fluctuations due to measurement or input uncertainties, and C' represents stochastic fluctuations.

Note: Most models do not attempt to estimate the stochastic fluctuations. Ensemble forecasts simulate the effects of $\Delta C_p'$, not C_p'.

Note: $\Delta C_p'$ has mostly to do with not satisfying the model's assumptions (grid/volume averages), which is commonly referred to as 'representativeness.'

My answer: We need an evaluation procedure, that uses statistical evaluation test methods to:

- Determine which of several models in performing best (for the data available) the physics within the model:
  - This will be defined as the "best performer."
- Determine whether the differences seen in the performance of the other models is statistically significant (in light of stochastic variations present in the data comparisons).
  - This will identify other models that may be performing as well (a set of 'best' performers).
- I call this the Olympics "High Bar"Analogy. This is an open (hopefully fair) competition, in which the rules are known and the conclusions reached are objectively determined.

My answer: (cont.)

- Once the 'set of best performers' has been defined, then a new set of statistical evaluation test methods would be used to determine, which of these models best performs the user-defined tasks.
  - Again, define the 'best' performer.
  - Then, test to see if differences in performance are statistically significant.
- This sequence recognizes that models are used for situations for which they do not have the requisite physics.
- If you test ONLY for the user defined tasks, you likely will end up with perverted models whose results are "tuned" to the data at hand, that may well provide erroneous results when used operationally.
- **Example**: Pasquill dispersion sigmas have a 3-minute averaging time. They are tested in their ability to replicate 1-hr, 3-hr concentration extremes, and then applied to produce annual averages.

Promising Test methods:

- Grouped Data:
  - (Irwin and Smith, 1984), ASTM (2000).
- Decomposed Time Series:
  - Eskridge, R.E., Ku, J.Y., Rao, S.T., Porter,P.S., Zurbenko, I.G., (1997)BAMS (78):1473-1483.
  - Rao, S.T., Zurbenko, I.G., Neagu, R., Porter, P.S., Ku, J.Y., Henry, R.F., (1997), BAMS, (78):2153-2166
- Process Analysis:
  - Dennis R.L. (1986), Air Pollution Modeling and its Application V, Plenum Press, pp. 411.-424.
  - Dennis, R.L., Arnold, J.R., Tonnesen, G.S., Y. Li (1999): Computer Physics Communications, 117:99-112.

All Models of Physical Processes are Cartoons of Reality

- **Models Simulate Only a Portion of the Natural Variability. They Do Not Simulate What Is Directly Seen.**
- **FIRST:** Test a Model to Accurately Perform the Physics Within It
- **THEN:** Test a Model to Perform Some User-defined Task (Which More Often Then Not Is Beyond the Capabilities of the Physics Within the Model).
- All "test methods" should provide a test of whether differences between several models are statistically significant.
- All "test methods" and test data sets should be peer reviewed and public domain.

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Clarke, J.F. (1964): A Simple Diffusion Model for Calculating Point Concentrations from Multiple Sources. *Journal of the Air Pollution Control Association*, 14(9):347-352

Hanna, S.R.; Chang, J.C., and Fernau, M.E., (1998): Monte Carlo Estimates of Uncertainties in Predictions by a Photochemical Grid Model (UAM-IV) Due to Uncertainties in Input Variables, *Atmospheric Environment*, Vol. 32, pp. 3617-3628.

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U.S. Environmental Protection Agency (1978b, 1986, 1987, 1995): *Guideline on Air Quality Models*. EPA-450/2-78-027, [This Guideline has been updated several time: 1986 as EPA-450/2-78-027R; 1987 as EPA/450/2-78/027R-SUPPL-A; 1993 as EPA-450/2-78-027R-B, and 1995 it was updated and incorporated into Appendix W to 40 CFR Part 51], U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards. Research Triangle Park, NC 27711.

Weil, J.C., Sykes, R.I., and Venkatram, A., (1992): Evaluating air quality models: review and outlook. *Journal of Applied Meteorology*, (31):1121-1145.